Distribution of Eigenvalues in Electromagnetic Scattering on an Arbitrarily Shaped Dielectric

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We study the distribution of eigenvalues for the Green operator occurring in the scattering of electromagnetic waves by an arbitrarily shaped dielectric medium. It is revealed that the totality of eigenvalues (counting multiplicities) can be enumerated as a sequence $\{\lambda_s\}_{s=1}^N, N\leq\aleph_0$, with only two possible accumulation points $\{0,-1/2\}$, and the following spectral series converges: $\sum_{s=1}^N|\lambda_s|^2|1+2\lambda_s|^4<+\infty$.

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1. INTRODUCTION

In [Ref. 1, Chap. 4], we studied the analytic properties of the Born equation for electromagnetic scattering:

$$(1+\chi)\boldsymbol{E}(\boldsymbol{r})-\chi\nabla\times\nabla\times\iiint_V\frac{\boldsymbol{E}(\boldsymbol{r}')e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}^3\boldsymbol{r}'=\boldsymbol{E}_{\mathrm{inc}}(\boldsymbol{r}),\quad \boldsymbol{r}\in V. \tag{1}$$

Here, the bounded open set $V\Subset\mathbb{R}^3$ represents the dielectric volume occupied by a homogeneous dielectric medium with complex susceptibility $\chi=\epsilon_r-1$, where ϵ_r is the relative dielectric permittivity, $n=\sqrt{\epsilon_r}$ the complex refractive index. We require that the boundary surface ∂V be smooth and the exterior volume $\mathbb{R}^3\setminus(V\cup\partial V)$ be connected, but the shape of V can be otherwise arbitrary. The (real part of the) complex-valued incident field $\boldsymbol{E}_{\mathrm{inc}}(\boldsymbol{r})e^{ickt},\boldsymbol{r}\in V$ represents a light beam oscillating in the fixed angular frequency $\omega=ck$, where c is the speed of light. Here, the time-harmonic factor e^{ickt} will be conveniently suppressed hereafter. The dielectric response (total electric field) inside the volume V is given by $\boldsymbol{E}(\boldsymbol{r}),\boldsymbol{r}\in V$. We abbreviate Eq. 1 as $(\hat I-\chi\hat{\mathscr G})\boldsymbol{E}=\boldsymbol{E}_{\mathrm{inc}}$, with $\hat I$ being the identity operator, and $\hat{\mathscr G}$ the Green operator.

It is a physical requirement that both $\boldsymbol{E}$ and $\boldsymbol{E}_{\mathrm{inc}}$ be square integrable and divergence-free. Therefore, we will pose the Born equation $(\hat I-\chi\hat{\mathscr G})\boldsymbol{E}=\boldsymbol{E}_{\mathrm{inc}}$ (Eq. 1) on a physical Hilbert space $\Phi(V;\mathbb{C}^3)=\mathrm{Cl}(C^\infty(V;\mathbb{C}^3)\cap\ker(\nabla\cdot)\cap L^2(V;\mathbb{C}^3))$, which is the L^2-closure of the totality of smooth, divergence-free and square-integrable complex-valued vector fields. [cf. Ref. 1, Chap. 4] The physical spectrum $\sigma^\Phi(\hat{\mathscr G})$ of the Green operator $\hat{\mathscr G}:\Phi(V;\mathbb{C}^3)\longrightarrow\Phi(V;\mathbb{C}^3)$ is the totality of complex numbers $\lambda\in\mathbb{C}$ that forbid a bounded inverse of the operator $\lambda\hat I-\hat{\mathscr G}:\Phi(V;\mathbb{C}^3)\longrightarrow\Phi(V;\mathbb{C}^3)$. Practically speaking, a point in the physical spectrum points to an "optical resonance mode" where the energy amplification ratio $\iiint_V|\boldsymbol{E}(\boldsymbol{r})|^2\,\mathrm{d}^3\boldsymbol{r}/\iiint_V|\boldsymbol{E}_{\mathrm{inc}}(\boldsymbol{r})|^2\,\mathrm{d}^3\boldsymbol{r}$ goes without bound.

We have proved, in [Ref. 1, Chap. 4], the following theorem regarding the topological structure of the physical spectrum $\sigma^\Phi(\hat{\mathscr G})$.

Theorem 1.1 (Compact Polynomial and Optical Resonance) *The non-compact Green operator $\hat{\mathscr G}:\Phi(V;\mathbb{C}^3)\longrightarrow\Phi(V;\mathbb{C}^3)$ is polynomially compact, with minimal polynomial $\hat{\mathscr G}(1+2\hat{\mathscr G})/2$.*

Moreover, $\sigma^\Phi(\hat{\mathscr G})$ is the union of the continuous spectrum $\sigma^\Phi_c(\hat{\mathscr G})=\{0,-1/2\}$ with the point spectrum $\sigma^\Phi_p(\hat{\mathscr G})$ that contains countably many eigenvalues. Each eigenvalue has a strictly negative imaginary part,[1] and is associated with a finite-dimensional eigenspace. The continuous spectrum $\sigma^\Phi_c(\hat{\mathscr G})=\{0,-1/2\}$ forms the only possible accumulation points of eigenvalues.

The shape-independent singularity $-1/2\in\sigma^\Phi_c(\hat{\mathscr G})$ corresponds to a universal optical resonance at susceptibility $\chi=-2$, i.e. relative permittivity $\epsilon_r=-1$. ∎

In this work, we will provide more detailed information regarding the spectral structure of $\hat{\mathscr G}:\Phi(V;\mathbb{C}^3)\longrightarrow\Phi(V;\mathbb{C}^3)$ by proving the following theorem.

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[1] The connectedness of $\mathbb{R}^3\setminus(V\cup\partial V)$ is conducive to ruling out real-valued eigenvalues, as well as confirming that $0\in\sigma^\Phi_c(\hat{\mathscr G})$. Even when $\mathbb{R}^3\setminus(V\cup\partial V)$ is not connected, the smooth dielectric boundary ∂V is strong enough to ensure the compactness of $\hat{\mathscr G}(\hat I+2\hat{\mathscr G}):\Phi(V;\mathbb{C}^3)\longrightarrow\Phi(V;\mathbb{C}^3)$.

Theorem 1.2 (Hilbert-Schmidt Polynomial and Spectral Series) *The operator $\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}})^2:\Phi(V;\mathbb{C}^3)\longrightarrow\Phi(V;\mathbb{C}^3)$ is of Hilbert-Schmidt type, and we have a convergent spectral series*[2]

$$\sum_{\lambda\in\sigma^{\Phi}(\hat{\mathscr{G}})}|\lambda|^2|1+2\lambda|^4<+\infty,$$

where the sum respects multiplicities in eigenvalues. ∎

Theorem 1.2 refines Theorem 1.1 by providing more quantitative details about the structure of the physical spectrum $\sigma^{\Phi}(\hat{\mathscr{G}})$. While $\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}})$ is already compact, it takes another factor of $(\hat{I}+2\hat{\mathscr{G}})$ to yield a Hilbert-Schmidt operator $\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}})^2$. While both the point $\{0\}$ and $\{-1/2\}$ can function as accumulation points in the spectrum $\sigma^{\Phi}(\hat{\mathscr{G}})$, the two distinct powers $|\lambda|^2$ and $|1+2\lambda|^4$ occurring in the convergent spectral series indicate different levels of eigenvalue aggregation surrounding the two accumulation points.

This article is organized as follows: §2 sketches the proof of polynomial compactness for $\hat{\mathscr{G}}:\Phi(V;\mathbb{C}^3)\longrightarrow\Phi(V;\mathbb{C}^3)$, thereby recapitulating the key ingredients of Theorem 1.1 and providing some analytic motivations for Theorem 1.2; §3 gives a detailed proof of Theorem 1.2, by extending the thoughts debriefed in §2; §4 provides some concrete examples that verify Theorem 1.2 and discusses its physical interpretation as well as possible applications.

2. POLYNOMIAL COMPACTNESS OF THE GREEN OPERATOR $\hat{\mathscr{G}}$

The Born equation (Eq. 1) is a strongly singular integral equation (with integral kernel behavior $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-3})$ and the Green operator $\hat{\mathscr{G}}$ is not compact. Nonetheless, the Green operator $\hat{\mathscr{G}}$ can be naturally decomposed into a sum of a Hermitian operator and a compact operator as $\hat{\mathscr{G}}=(\hat{\mathscr{G}}-\hat{\gamma})+\hat{\gamma}$. Here, the Hermitian operator $\hat{\mathscr{G}}-\hat{\gamma}$ is given by

$$((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}):=\nabla\left[\nabla\cdot\iiint_V\frac{\boldsymbol{E}(\boldsymbol{r}')}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}^3\boldsymbol{r}'\right]$$

and the compact operator $\hat{\gamma}$ is defined as

$$(\hat{\gamma}\boldsymbol{E})(\boldsymbol{r}):=\nabla\times\nabla\times\iiint_V\frac{\boldsymbol{E}(\boldsymbol{r}')(e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}-1)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}^3\boldsymbol{r}'. \tag{2}$$

Physically speaking, the operator $\hat{\mathscr{G}}-\hat{\gamma}$ represents the long-wavelength limit $(2\pi/k\to+\infty)$ of electromagnetic scattering, which is just electrostatic induction; the operator $\hat{\gamma}$ represents "dynamic corrections" on top of the electrostatic picture. Mathematically speaking, the "static induction" operator $\hat{\mathscr{G}}-\hat{\gamma}$ is Hermitian, satisfying the inequality $0\geq\langle\boldsymbol{E},(\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E}\rangle_V\geq-\langle\boldsymbol{E},\boldsymbol{E}\rangle_V$ [Ref. 1, p. 188]; the "dynamic correction" operator $\hat{\gamma}$ is weakly singular, with only $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-1})$ divergence in the integral kernel [Ref. 1, p. 176], hence is qualified as a Hilbert-Schmidt operator, which is a special type of compact operator.

As the difference between the quadratic polynomial $\hat{\mathscr{G}}+2\hat{\mathscr{G}}^2$ and the expression $(\hat{\mathscr{G}}-\hat{\gamma})+2(\hat{\mathscr{G}}-\hat{\gamma})^2$ is evidently a compact operator, we only need to verify the following proposition before claiming the compactness of $\hat{\mathscr{G}}+2\hat{\mathscr{G}}^2$.

Proposition 2.1 *The expression $(\hat{\mathscr{G}}-\hat{\gamma})+2(\hat{\mathscr{G}}-\hat{\gamma})^2:\Phi(V;\mathbb{C}^3)\longrightarrow\Phi(V;\mathbb{C}^3)$ defines a compact operator.*

Proof (Sketch) A key observation is that, the "static induction" $\hat{\mathscr{G}}-\hat{\gamma}$ maps any $\boldsymbol{E}\in\Phi(V;\mathbb{C}^3)$ to

$$((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r})=-\nabla\left[\oiint_{\partial V}\frac{\boldsymbol{n}'\cdot\boldsymbol{E}(\boldsymbol{r}')}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}S'\right],$$

which is the gradient of a harmonic function, reminiscent of an electrostatic field. The bulk behavior $((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}),\boldsymbol{r}\in V$ ("electrostatic field") is fully determined by the boundary behavior of its normal component $\boldsymbol{n}\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}),\boldsymbol{r}\in\partial V$ ("boundary surface charge"), and this one-to-one correspondence is also robust in both directions [Ref. 2, p. 252]. Technically speaking, according to the boundary trace theorem and the robustness of Neumann boundary problems, there are two finite positive constants C_1 and C_2 such that

$$C_1\|(\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E}\|_{L^2(V;\mathbb{C}^3)}\leq\|\boldsymbol{n}\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})\|_{H^{-1/2}(\partial V;\mathbb{C})}\leq C_2\|(\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E}\|_{L^2(V;\mathbb{C}^3)}.$$

[2] The convergence remains true even when the exterior volume $\mathbb{R}^3\setminus(V\cup\partial V)$ is not connected.

The compactness of the polynomial $(\hat{\mathscr{G}}-\hat{\gamma})+2(\hat{\mathscr{G}}-\hat{\gamma})^2$ on $\Phi(V;\mathbb{C}^3)$ is then evident from the boundary integral representation

$$\boldsymbol{n}\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r})+2\boldsymbol{n}\cdot((\hat{\mathscr{G}}-\hat{\gamma})^2\boldsymbol{E})(\boldsymbol{r})=-2\oiint_{\partial V}\boldsymbol{n}'\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}')(\boldsymbol{n}\cdot\nabla)\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}S',\quad \boldsymbol{r}\in\partial V \tag{3}$$

where the integral kernel $(\boldsymbol{n}\cdot\nabla)(4\pi|\boldsymbol{r}-\boldsymbol{r}'|)^{-1}=O(|\boldsymbol{r}-\boldsymbol{r}'|^{-1})$ is weakly singular (see [Ref. 3, p. 48] or [Ref. 4]), hence induces a compact operator (cf. [Ref. 4] or [Ref. 5, p. 124]) on $H^{-1/2}(\partial V;\mathbb{C})$. Here, the choice of the coefficient 2 in the quadratic term of $(\hat{\mathscr{G}}-\hat{\gamma})+2(\hat{\mathscr{G}}-\hat{\gamma})^2$ is critical, in that

$$\begin{aligned}&\lim_{\varepsilon\to0^+}(\boldsymbol{n}\cdot\nabla)\oiint_{\partial V}\boldsymbol{n}'\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}')\frac{1}{4\pi|\boldsymbol{r}-\varepsilon\boldsymbol{n}-\boldsymbol{r}'|}\,\mathrm{d}S'\\&=\oiint_{\partial V}\boldsymbol{n}'\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}')(\boldsymbol{n}\cdot\nabla)\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}S'+\frac{1}{2}\boldsymbol{n}\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}),\quad \boldsymbol{r}\in\partial V.\end{aligned}$$

(Here, the limit is interpreted in the sense of boundary trace.) In other words, the construction of the quadratic polynomial ensures that the non-compact ingredients cancel out. ∎

In the next short lemma, we will derive a volume integral analog of Eq. 3, after introducing the notations for electrostatic Green functions. The Green function $G_D(\boldsymbol{r},\boldsymbol{r}')$ with Dirichlet boundary condition is given by the unique solution to

$$\nabla^2G_D(\boldsymbol{r},\boldsymbol{r}')=-\delta(\boldsymbol{r}-\boldsymbol{r}'),\quad \boldsymbol{r},\boldsymbol{r}'\in V;\qquad G_D(\boldsymbol{r},\boldsymbol{r}')=0,\quad \boldsymbol{r}\in V,\boldsymbol{r}'\in\partial V.$$

The Green function thus defined automatically honors reciprocal symmetry $G_D(\boldsymbol{r},\boldsymbol{r}')=G_D(\boldsymbol{r}',\boldsymbol{r})$ [Ref. 6, p. 40]. Customarily, the Green function $G_N(\boldsymbol{r},\boldsymbol{r}')$ with Neumann boundary condition is prescribed as a solution to

$$\nabla^2G_N(\boldsymbol{r},\boldsymbol{r}')=-\delta(\boldsymbol{r}-\boldsymbol{r}'),\quad \boldsymbol{r},\boldsymbol{r}'\in V;\qquad (\boldsymbol{n}'\cdot\nabla')G_N(\boldsymbol{r},\boldsymbol{r}')=-\frac{1}{\oiint_{\partial V}\mathrm{d}S'},\quad \boldsymbol{r}\in V,\boldsymbol{r}'\in\partial V.$$

Hereafter, we will impose the constraint of reciprocal symmetry to the Green function $G_N(\boldsymbol{r},\boldsymbol{r}')=G_N(\boldsymbol{r}',\boldsymbol{r})$ (see [Ref. 7] or [Ref. 6, p. 40] for such feasibility).

Lemma 2.1 *Define*

$$\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}'):=G_D(\boldsymbol{r},\boldsymbol{r}')+G_N(\boldsymbol{r},\boldsymbol{r}')-\frac{1}{2\pi|\boldsymbol{r}-\boldsymbol{r}'|},\quad \boldsymbol{r},\boldsymbol{r}'\in V,$$

which is a harmonic function with respect to both $\boldsymbol{r}$ *and* $\boldsymbol{r}'$*, then we have the volume integral representation*

$$((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r})+2((\hat{\mathscr{G}}-\hat{\gamma})^2\boldsymbol{E})(\boldsymbol{r})=\iiint_V\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}',\quad \boldsymbol{r}\in V, \tag{4}$$

where $\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$ *is a* 3×3 *matrix filled with mixed second-order derivatives of* $\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$*.*

Proof By properties of the Green functions, we have

$$\begin{aligned}\iiint_V\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}'&=\nabla\oiint_{\partial V}\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{n}'\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}')\,\mathrm{d}S'\\&=\nabla\oiint_{\partial V}G_N(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{n}'\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}')\,\mathrm{d}S'-2\nabla\oiint_{\partial V}\frac{\boldsymbol{n}'\cdot((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}')}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}S'\\&=((\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E})(\boldsymbol{r}')+2((\hat{\mathscr{G}}-\hat{\gamma})^2\boldsymbol{E})(\boldsymbol{r}),\quad \boldsymbol{r}\in V,\end{aligned}$$

as claimed in Eq. 4. ∎

From the above arguments, it is straightforward to check that the integral kernel $\hat{K}_1(\boldsymbol{r},\boldsymbol{r}'):=\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$ is Hermitian $\hat{K}_1^*(\boldsymbol{r},\boldsymbol{r}')=\hat{K}_1(\boldsymbol{r}',\boldsymbol{r})$, where an asterisk denotes the conjugate transpose of a 3×3 matrix. What we have proved in Proposition 2.1 is that the integral kernel $\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$ induces a compact linear operator, unlike the strongly singular integral kernel associated with the non-compact operator $\hat{\mathscr{G}}$. In the next section, we will show that the following integral kernel (where products represent matrix multiplications)

$$\iiint_V\nabla\nabla''\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}'')\nabla''\nabla'\mathfrak{g}(\boldsymbol{r}'',\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}''=\iiint_V\hat{K}_1(\boldsymbol{r},\boldsymbol{r}'')\hat{K}_1(\boldsymbol{r}'',\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}''$$

is square-integrable, so it induces a Hilbert-Schmidt operator, just as the "dynamic correction" operator $\hat{\gamma}$.

3. HILBERT-SCHMIDT POLYNOMIAL IN THE GREEN OPERATOR $\hat{\mathscr{G}}$

According to the Schur-Weyl inequality (see [Refs. 8, 9], also [Ref. 10, p. 8]), we have

$$\sqrt{\sum_{\lambda\in\sigma^{\Phi}(\hat{\mathscr{G}})}|\lambda|^2|1+2\lambda|^4}\le\|\hat{\mathscr{G}}(\hat I+2\hat{\mathscr{G}})^2\|_2:=\sqrt{\sum_{s=1}^{\infty}\|\hat{\mathscr{G}}(\hat I+2\hat{\mathscr{G}})^2\boldsymbol{e}_s\|^2_{L^2(V;\mathbb{C}^3)}}$$

where $\{\boldsymbol{e}_s|s=1,2,\dots\}$ is any complete set of orthonormal basis for the Hilbert space $\Phi(V;\mathbb{C}^3)$, so the Hilbert-Schmidt bound $\|\hat{\mathscr{G}}(\hat I+2\hat{\mathscr{G}})^2\|_2<+\infty$ would entail the convergence of the spectral series in question. Using the inequalities $\|\hat A\hat B\|_2\le\|\hat A\|_2\|\hat B\|$ and $\|\hat B\hat A\|_2\le\|\hat A\|_2\|\hat B\|$ [Ref. 11, p. 218], together with the facts that $\|\hat{\mathscr{G}}-\hat\gamma\|\le1$, $\|\hat I+\hat{\mathscr{G}}-\hat\gamma\|\le1$ and $\|\hat\gamma\|\le\|\hat\gamma\|_2<+\infty$, we may deduce the inequality

$$\begin{aligned}&\|(\hat I+2\hat{\mathscr{G}})^2\hat{\mathscr{G}}\|_2\\ \le{}&\|(\hat I+2\hat{\mathscr{G}}-2\hat\gamma)^2(\hat{\mathscr{G}}-\hat\gamma)\|_2\\ &+\|\hat\gamma+4[(\hat{\mathscr{G}}-\hat\gamma)\hat\gamma+\hat\gamma(\hat{\mathscr{G}}-\hat\gamma)](\hat I+\hat{\mathscr{G}}-\hat\gamma)+4(\hat{\mathscr{G}}-\hat\gamma)^2\hat\gamma+4(\hat I+\hat{\mathscr{G}}-\hat\gamma)\hat\gamma^2+4\hat\gamma(\hat{\mathscr{G}}-\hat\gamma)\hat\gamma+4\hat\gamma^2(\hat{\mathscr{G}}-\hat\gamma)^2+4\hat\gamma^3\|_2\\ \le{}&\|(\hat I+2\hat{\mathscr{G}}-2\hat\gamma)^2(\hat{\mathscr{G}}-\hat\gamma)\|_2+\|\hat\gamma\|_2(13+12\|\hat\gamma\|+4\|\hat\gamma\|^2).\end{aligned}\tag{5}$$

Therefore, the major task in Theorem 1.2 boils down to an analysis of the action of $(\hat I+2\hat{\mathscr{G}}-2\hat\gamma)^2$ on the range of $(\hat{\mathscr{G}}-\hat\gamma)$, which is represented by the integral kernel

$$\iiint_V\nabla\nabla''\mathfrak{g}(\boldsymbol r,\boldsymbol r'')\nabla''\nabla'\mathfrak{g}(\boldsymbol r'',\boldsymbol r')\,\mathrm{d}^3\boldsymbol r''.$$

Before establishing the Hilbert-Schmidt bound for the operator $(\hat I+2\hat{\mathscr{G}}-2\hat\gamma)^2(\hat{\mathscr{G}}-\hat\gamma)$ in Proposition 3.1, we explore the boundary behavior of the integral kernel $\mathfrak{g}(\boldsymbol r,\boldsymbol r')$ in the lemma below.

Lemma 3.1 *For any $f\in H^{-1/2}(\partial V;\mathbb{C})$, we have the following limits in the sense of boundary trace:*

$$\lim_{\varepsilon\to0^+}\oiint_{\partial V}f(\boldsymbol r')(\boldsymbol n'\cdot\nabla')\mathfrak{g}(\boldsymbol r-\varepsilon\boldsymbol n,\boldsymbol r')\,\mathrm{d}S'=-\oiint_{\partial V}f(\boldsymbol r')\left[(\boldsymbol n'\cdot\nabla')\frac{1}{2\pi|\boldsymbol r-\boldsymbol r'|}+\frac{1}{\oiint_{\partial V}\mathrm{d}S}\right]\mathrm{d}S';\tag{$*$}$$

$$\lim_{\varepsilon\to0^+}(\boldsymbol n\cdot\nabla)\oiint_{\partial V}\mathfrak{g}(\boldsymbol r-\varepsilon\boldsymbol n,\boldsymbol r')f(\boldsymbol r')\,\mathrm{d}S'=-\oiint_{\partial V}f(\boldsymbol r')\left[(\boldsymbol n\cdot\nabla)\frac{1}{2\pi|\boldsymbol r-\boldsymbol r'|}+\frac{1}{\oiint_{\partial V}\mathrm{d}S}\right]\mathrm{d}S',\tag{$**$}$$

where $\boldsymbol r\in\partial V$.

Proof We first prove $(*)$ by computing

$$\begin{aligned}&\lim_{\varepsilon\to0^+}\oiint_{\partial V}f(\boldsymbol r')(\boldsymbol n'\cdot\nabla')\mathfrak{g}(\boldsymbol r-\varepsilon\boldsymbol n,\boldsymbol r')\,\mathrm{d}S'\\ ={}&\lim_{\varepsilon\to0^+}\oiint_{\partial V}f(\boldsymbol r')(\boldsymbol n'\cdot\nabla')G_D(\boldsymbol r-\varepsilon\boldsymbol n,\boldsymbol r')\,\mathrm{d}S'-\frac{1}{\oiint_{\partial V}\mathrm{d}S}\oiint_{\partial V}f(\boldsymbol r')\,\mathrm{d}S'-2\lim_{\varepsilon\to0^+}\oiint_{\partial V}f(\boldsymbol r')(\boldsymbol n'\cdot\nabla')\frac{1}{4\pi|\boldsymbol r-\varepsilon\boldsymbol n-\boldsymbol r'|}\,\mathrm{d}S'\\ ={}&-f(\boldsymbol r')-\frac{1}{\oiint_{\partial V}\mathrm{d}S}\oiint_{\partial V}f(\boldsymbol r')\,\mathrm{d}S'-2\lim_{\varepsilon\to0^+}\oiint_{\partial V}f(\boldsymbol r')(\boldsymbol n'\cdot\nabla')\frac{1}{4\pi|\boldsymbol r-\varepsilon\boldsymbol n-\boldsymbol r'|}\,\mathrm{d}S'\\ ={}&-\oiint_{\partial V}f(\boldsymbol r')\left[(\boldsymbol n'\cdot\nabla')\frac{1}{2\pi|\boldsymbol r-\boldsymbol r'|}+\frac{1}{\oiint_{\partial V}\mathrm{d}S}\right]\mathrm{d}S',\quad\boldsymbol r\in V,\end{aligned}$$

where we have invoked the solution to the Dirichlet boundary value problem using G_D, and the Neumann boundary condition for G_N. To tackle $(**)$, we perform the following analysis:

$$\begin{aligned}&\lim_{\varepsilon\to0^+}(\boldsymbol n\cdot\nabla)\oiint_{\partial V}\mathfrak{g}(\boldsymbol r-\varepsilon\boldsymbol n,\boldsymbol r')f(\boldsymbol r')\,\mathrm{d}S'\\ ={}&\lim_{\varepsilon\to0^+}(\boldsymbol n\cdot\nabla)\oiint_{\partial V}\left[G_N(\boldsymbol r-\varepsilon\boldsymbol n,\boldsymbol r')-\frac{1}{2\pi|\boldsymbol r-\varepsilon\boldsymbol n-\boldsymbol r'|}\right]f(\boldsymbol r')\,\mathrm{d}S'\\ ={}&\lim_{\varepsilon\to0^+}(\boldsymbol n\cdot\nabla)\oiint_{\partial V}G_N(\boldsymbol r-\varepsilon\boldsymbol n,\boldsymbol r')\left[f(\boldsymbol r)-\frac{\oiint_{\partial V}f(\boldsymbol r'')\,\mathrm{d}S''}{\oiint_{\partial V}\mathrm{d}S}\right]\mathrm{d}S'+\frac{\oiint_{\partial V}f(\boldsymbol r'')\,\mathrm{d}S''}{\oiint_{\partial V}\mathrm{d}S}\lim_{\varepsilon\to0^+}(\boldsymbol n\cdot\nabla)\oiint_{\partial V}G_N(\boldsymbol r-\varepsilon\boldsymbol n,\boldsymbol r')\,\mathrm{d}S'\\ &-2\lim_{\varepsilon\to0^+}\oiint_{\partial V}f(\boldsymbol r')(\boldsymbol n\cdot\nabla)\frac{1}{4\pi|\boldsymbol r-\varepsilon\boldsymbol n-\boldsymbol r'|}\,\mathrm{d}S'\\ ={}&-\oiint_{\partial V}f(\boldsymbol r')\left[(\boldsymbol n\cdot\nabla)\frac{1}{2\pi|\boldsymbol r-\boldsymbol r'|}+\frac{1}{\oiint_{\partial V}\mathrm{d}S}\right]\mathrm{d}S',\quad\boldsymbol r\in\partial V,\end{aligned}$$

where we have relied on the homogeneous Dirichlet boundary condition for G_D, the solution to the Neumann boundary value problem in terms of G_N, and the fact that

$$\begin{aligned}
&\lim_{\varepsilon\to0^+}(\boldsymbol{n}\cdot\nabla)\oiint_{\partial V}G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}')\,\mathrm{d}S'\\
&=\lim_{\delta\to0^+}\lim_{\varepsilon\to0^+}(\boldsymbol{n}\cdot\nabla)\oiint_{\partial V}G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}'-\delta\boldsymbol{n}')\,\mathrm{d}S'+\lim_{\delta\to0^+}\lim_{\varepsilon\to0^+}(\boldsymbol{n}\cdot\nabla)\oiint_{\partial V}[G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}')-G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}'-\delta\boldsymbol{n}')]\,\mathrm{d}S'\\
&=-1+\lim_{\delta\to0^+}\lim_{\varepsilon\to0^+}(\boldsymbol{n}\cdot\nabla)\oiint_{\partial V}[G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}')-G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}'-\delta\boldsymbol{n}')]\,\mathrm{d}S'=0.
\end{aligned}$$

Here, the last line can be justified as follows. For sufficiently small $\delta>0$, we may define the boundary layer of thickness δ as $V^-_{(\delta)}:=\{\boldsymbol{r}\in V|\operatorname{dist}(\boldsymbol{r},\partial V)<\delta\}$, so that the function $\operatorname{dist}(\boldsymbol{r},\partial V):=\min_{\boldsymbol{r}'\in\partial V}|\boldsymbol{r}-\boldsymbol{r}'|$ is smooth in $\boldsymbol{r}\in V^-_{(\delta)}\cup\partial V^-_{(\delta)}$, satisfying $(\boldsymbol{n}\cdot\nabla)\operatorname{dist}(\boldsymbol{r},\partial V)=-1$. Thus, choosing $\boldsymbol{v}'$ as the outward normal of the smooth domain $V^-_{(\delta)}$, we have

$$\begin{aligned}
&\lim_{\delta\to0^+}\lim_{\varepsilon\to0^+}(\boldsymbol{n}\cdot\nabla)\oiint_{\partial V}[G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}')-G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}'-\delta\boldsymbol{n}')]\,\mathrm{d}S'\\
&=\lim_{\delta\to0^+}\lim_{\varepsilon\to0^+}(\boldsymbol{n}\cdot\nabla)\oiint_{\partial V^-_{(\delta)}}[\operatorname{dist}(\boldsymbol{r}',\partial V)(\boldsymbol{v}'\cdot\nabla')G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}')-G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}')(\boldsymbol{v}'\cdot\nabla')\operatorname{dist}(\boldsymbol{r}',\partial V)]\,\mathrm{d}S'\\
&=\lim_{\delta\to0^+}\lim_{\varepsilon\to0^+}(\boldsymbol{n}\cdot\nabla)\iiint_{V^-_{(\delta)}}[\operatorname{dist}(\boldsymbol{r}',\partial V)\nabla'^2G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}')-G_N(\boldsymbol{r}-\varepsilon\boldsymbol{n},\boldsymbol{r}')\nabla'^2\operatorname{dist}(\boldsymbol{r}',\partial V)]\,\mathrm{d}^3\boldsymbol{r}'\\
&=-\lim_{\delta\to0^+}\lim_{\varepsilon\to0^+}(\boldsymbol{n}\cdot\nabla)\operatorname{dist}(\boldsymbol{r}-\varepsilon\boldsymbol{n},\partial V)=1.\quad\blacksquare
\end{aligned}$$

Now, for fixed $\boldsymbol{r}'\in\partial V$, the boundary trace $(\boldsymbol{n}\cdot\nabla)\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$, as a function of $\boldsymbol{r}\in\partial V$, has merely a weak singularity $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-1})$, hence $(\boldsymbol{n}\cdot\nabla)\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\in H^{-1/2}_{\boldsymbol{r}}(\partial V;\mathbb{C})$. As a result, in the independent variable $\boldsymbol{r}$, the harmonic vector field $\nabla\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\in L^2_{\boldsymbol{r}}(V;\mathbb{C}^3)$ is square integrable, i.e. $\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\in W^{1,2}_{\boldsymbol{r}}(V;\mathbb{C})$ for all boundary points $\boldsymbol{r}'\in\partial V$. Furthermore, $\sup_{\boldsymbol{r}'\in\partial V}\iiint_V|\nabla\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')|^2\,\mathrm{d}^3\boldsymbol{r}$ is finite. The boundary trace mapping from the Sobolev space $W^{1,2}(V;\mathbb{C})$ to $H^{1/2}(\partial V;\mathbb{C})$ then leads to $\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\in H^{1/2}_{\boldsymbol{r}}(\partial V;\mathbb{C}),\boldsymbol{r}'\in\partial V$. Moreover, the expression $\iiint_V|\nabla\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')|^2\,\mathrm{d}^3\boldsymbol{r}$ defines a subharmonic function in $\boldsymbol{r}'$, which may only attain its maximum at the boundary $\boldsymbol{r}'\in\partial V$. Therefore, the condition $\sup_{\boldsymbol{r}'\in\partial V}\iiint_V|\nabla\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')|^2\,\mathrm{d}^3\boldsymbol{r}<+\infty$ entails the square integrability of $\nabla\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\in L^2_{\boldsymbol{r}}(V;\mathbb{C}^3),\boldsymbol{r}'\in V$. As a result, we always have $\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\in H^{1/2}_{\boldsymbol{r}}(\partial V;\mathbb{C})$, no matter the point $\boldsymbol{r}'$ is at the boundary $\boldsymbol{r}'\in\partial V$ or in the interior $\boldsymbol{r}'\in V$.

Proposition 3.1 *The operator $(\hat I+2\hat{\mathscr G}-2\hat\gamma)^2(\hat{\mathscr G}-\hat\gamma):\Phi(V;\mathbb{C}^3)\longrightarrow\Phi(V;\mathbb{C}^3)$ is of Hilbert-Schmidt type.*

Proof Without loss of generality, we may pick the complete orthonormal basis set $\{\boldsymbol{e}_s|s=1,2,\dots\}\subset\Phi(V;\mathbb{C}^3)$ so that one of its subset $\{\boldsymbol{f}_s|s=1,2,\dots\}$ exhausts all the eigenvectors subordinate to the non-zero eigenvalues of the polynomially compact Hermitian operator $\hat{\mathscr G}-\hat\gamma:\Phi(V;\mathbb{C}^3)\longrightarrow\Phi(V;\mathbb{C}^3)$. The bound on the operator norm $\|\hat{\mathscr G}-\hat\gamma\|\le1$ then naturally leads to

$$\|(\hat I+2\hat{\mathscr G}-2\hat\gamma)^2(\hat{\mathscr G}-\hat\gamma)\|_2\le\sqrt{\sum_{s=1}^\infty\|(\hat I+2\hat{\mathscr G}-2\hat\gamma)^2\boldsymbol{f}_s\|^2_{L^2(V;\mathbb{C}^3)}}.$$

In the formula above, each $\boldsymbol{f}_s$ is the gradient of a harmonic function, so the following integral representations hold for $\boldsymbol{F}\in\operatorname{Cl}\operatorname{span}\{\boldsymbol{f}_s|s=1,2,\dots\}$:

$$\begin{aligned}
((\hat I+2\hat{\mathscr G}-2\hat\gamma)\boldsymbol{F})(\boldsymbol{r})&=\iiint_V\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{F}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}'=\iiint_V\hat K_1(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{F}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}',\\
((\hat I+2\hat{\mathscr G}-2\hat\gamma)^2\boldsymbol{F})(\boldsymbol{r})&=\iiint_V\nabla\nabla'\mathfrak{G}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{F}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}'=\iiint_V\hat K_2(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{F}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}',
\end{aligned}$$

where

$$\mathfrak{G}(\boldsymbol{r},\boldsymbol{r}'):=\iiint_V\nabla''\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}'')\cdot\nabla''\mathfrak{g}(\boldsymbol{r}'',\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}''$$

evidently satisfies the harmonic equations $\nabla^2\mathfrak{G}(\boldsymbol{r},\boldsymbol{r}')=0$ and $\nabla'^2\mathfrak{G}(\boldsymbol{r},\boldsymbol{r}')=0$ for $\boldsymbol{r},\boldsymbol{r}'\in V$.

Now, extending the action of the integral kernel $\hat K_2(\boldsymbol{r},\boldsymbol{r}')$ on $\{\boldsymbol{f}_s|s=1,2,\dots\}\subset\Phi(V;\mathbb{C}^3)$ to a complete orthonormal basis set of $L^2(V;\mathbb{C}^3)$, and using the Parseval identity on $L^2(V;\mathbb{C}^3)$, we can show that

$$\sum_{s=1}^\infty\|(\hat I+2\hat{\mathscr G}-2\hat\gamma)^2\boldsymbol{f}_s\|^2_{L^2(V;\mathbb{C}^3)}=\iiint_V\left\{\iiint_V\operatorname{Tr}[\hat K_2^*(\boldsymbol{r},\boldsymbol{r}')\hat K_2(\boldsymbol{r},\boldsymbol{r}')]\,\mathrm{d}^3\boldsymbol{r}'\right\}\mathrm{d}^3\boldsymbol{r},\tag{6}$$

where "Tr" denotes the trace of a 3×3 matrix. To justify the equality in the above formula, we note that $\iiint_V \hat{K}_2(\boldsymbol r,\boldsymbol r')\boldsymbol F(\boldsymbol r')\,\mathrm d^3\boldsymbol r'$ represents the gradient of a harmonic function for whatever square-integrable input $\boldsymbol F\in L^2(V;\mathbb C^3)$, so every eigenvector $\boldsymbol F_\lambda\in L^2(V;\mathbb C^3)$ satisfying $\iiint_V \hat{K}_2(\boldsymbol r,\boldsymbol r')\boldsymbol F_\lambda(\boldsymbol r')\,\mathrm d^3\boldsymbol r'=\lambda\boldsymbol F_\lambda(\boldsymbol r),\lambda\neq 0$ must belong to the function space $\Phi(V;\mathbb C^3)$. In other words, the extension of the orthonormal basis set leaves the Hilbert-Schmidt norm intact.

We may go on to cast the volume integral representation of $\mathfrak G(\boldsymbol r,\boldsymbol r')$ into a surface integral (more precisely, a canonical pairing [Ref. 2, p. 206] between $\mathfrak g(\boldsymbol r,\boldsymbol r'')\in H^{1/2}_{\boldsymbol r''}(\partial V;\mathbb C)$ and $(\boldsymbol n''\cdot\nabla'')\mathfrak g(\boldsymbol r'',\boldsymbol r')\in H^{-1/2}_{\boldsymbol r''}(\partial V;\mathbb C)$) in two ways

$$\mathfrak G(\boldsymbol r,\boldsymbol r')=\oiint_{\partial V}\mathfrak g(\boldsymbol r,\boldsymbol r'')(\boldsymbol n''\cdot\nabla'')\mathfrak g(\boldsymbol r'',\boldsymbol r')\,\mathrm dS''=\oiint_{\partial V}\mathfrak g(\boldsymbol r'',\boldsymbol r')(\boldsymbol n''\cdot\nabla'')\mathfrak g(\boldsymbol r,\boldsymbol r'')\,\mathrm dS'',\quad \boldsymbol r,\boldsymbol r'\in V.$$

Clearly, the reciprocal symmetry $\mathfrak g(\boldsymbol r_1,\boldsymbol r_2)=\mathfrak g(\boldsymbol r_2,\boldsymbol r_1)$ entails the result $\mathfrak G(\boldsymbol r,\boldsymbol r')=\mathfrak G(\boldsymbol r',\boldsymbol r)$. Interpreting the expression $\mathfrak G(\boldsymbol r,\boldsymbol r'),\boldsymbol r\in V,\boldsymbol r'\in\partial V$ as a boundary trace (denoted by the limit notation "$\lim_{\varepsilon\to0^+}$" as before), we may use Lemma 3.1($*$) to deduce

$$\begin{aligned}\mathfrak G(\boldsymbol r,\boldsymbol r')&=\lim_{\varepsilon\to0^+}\oiint_{\partial V}\mathfrak g(\boldsymbol r,\boldsymbol r'')(\boldsymbol n''\cdot\nabla'')\mathfrak g(\boldsymbol r'',\boldsymbol r'-\varepsilon\boldsymbol n')\,\mathrm dS''\\&=-\oiint_{\partial V}\mathfrak g(\boldsymbol r,\boldsymbol r'')\left[(\boldsymbol n''\cdot\nabla'')\frac{1}{2\pi|\boldsymbol r'-\boldsymbol r''|}+\frac{1}{\oiint_{\partial V}\mathrm dS'}\right]\mathrm dS'',\quad \boldsymbol r\in V,\boldsymbol r'\in\partial V.\end{aligned}$$

Then, employing the harmonic equations for $\mathfrak G(\boldsymbol r,\boldsymbol r')$, we may convert the double volume integral on the right-hand side of Eq. 6 to a double surface integral in the following fashion:

$$\begin{aligned}\iiint_V\left\{\iiint_V\mathrm{Tr}[\hat K_2^*(\boldsymbol r,\boldsymbol r')\hat K_2(\boldsymbol r,\boldsymbol r')]\,\mathrm d^3\boldsymbol r'\right\}\mathrm d^3\boldsymbol r&=\iiint_V\sum_{\boldsymbol u\in\{\boldsymbol e_x,\boldsymbol e_y,\boldsymbol e_z\}}\left\{\iiint_V\sum_{\boldsymbol v\in\{\boldsymbol e_x,\boldsymbol e_y,\boldsymbol e_z\}}[(\boldsymbol u\cdot\nabla)(\boldsymbol v\cdot\nabla')\mathfrak G(\boldsymbol r,\boldsymbol r')]^2\,\mathrm d^3\boldsymbol r'\right\}\mathrm d^3\boldsymbol r\\&=\iiint_V\sum_{\boldsymbol u\in\{\boldsymbol e_x,\boldsymbol e_y,\boldsymbol e_z\}}\left\{\oiint_{\partial V}[(\boldsymbol u\cdot\nabla)\mathfrak G(\boldsymbol r,\boldsymbol r')][(\boldsymbol u\cdot\nabla)(\boldsymbol n'\cdot\nabla')\mathfrak G(\boldsymbol r,\boldsymbol r')]\,\mathrm dS'\right\}\mathrm d^3\boldsymbol r\\&=\oiint_{\partial V}\left\{\oiint_{\partial V}[(\boldsymbol n\cdot\nabla)\mathfrak G(\boldsymbol r,\boldsymbol r')][(\boldsymbol n'\cdot\nabla')\mathfrak G(\boldsymbol r,\boldsymbol r')]\,\mathrm dS'\right\}\mathrm dS.\end{aligned}\tag{7}$$

Here, the integrands in the last line are understood in terms of boundary trace, expressible as a specific case of Lemma 3.1($**$):

$$\begin{aligned}(\boldsymbol n\cdot\nabla)\mathfrak G(\boldsymbol r,\boldsymbol r')&=\lim_{\varepsilon\to0^+}(\boldsymbol n\cdot\nabla)\mathfrak G(\boldsymbol r-\varepsilon\boldsymbol n,\boldsymbol r')\\&=\oiint_{\partial V}\left[(\boldsymbol n\cdot\nabla)\frac{1}{2\pi|\boldsymbol r-\boldsymbol r''|}+\frac{1}{\oiint_{\partial V}\mathrm dS}\right]\left[(\boldsymbol n''\cdot\nabla'')\frac{1}{2\pi|\boldsymbol r'-\boldsymbol r''|}+\frac{1}{\oiint_{\partial V}\mathrm dS'}\right]\mathrm dS'',\quad\boldsymbol r,\boldsymbol r'\in\partial V.\end{aligned}$$

Judging from the surface integral above, the singular behavior of $(\boldsymbol n\cdot\nabla)\mathfrak G(\boldsymbol r,\boldsymbol r')$ is comparable to the convolution of two $O(|\boldsymbol r-\boldsymbol r'|^{-1})$ integral kernels on the boundary surface, which results in the short distance asymptotics $(\boldsymbol n\cdot\nabla)\mathfrak G(\boldsymbol r,\boldsymbol r')=O(\ln|\boldsymbol r-\boldsymbol r'|)$. Likewise, by reciprocal symmetry $\mathfrak G(\boldsymbol r,\boldsymbol r')=\mathfrak G(\boldsymbol r',\boldsymbol r)$, we have

$$(\boldsymbol n'\cdot\nabla')\mathfrak G(\boldsymbol r,\boldsymbol r')=(\boldsymbol n'\cdot\nabla')\mathfrak G(\boldsymbol r',\boldsymbol r)=\oiint_{\partial V}\left[(\boldsymbol n'\cdot\nabla')\frac{1}{2\pi|\boldsymbol r'-\boldsymbol r''|}+\frac{1}{\oiint_{\partial V}\mathrm dS'}\right]\left[(\boldsymbol n''\cdot\nabla'')\frac{1}{2\pi|\boldsymbol r-\boldsymbol r''|}+\frac{1}{\oiint_{\partial V}\mathrm dS}\right]\mathrm dS'',$$

which is again a surface integral kernel of order $O(\ln|\boldsymbol r-\boldsymbol r'|)$. As the logarithmic singularity is square integrable, the surface integral

$$\oiint_{\partial V}[(\boldsymbol n\cdot\nabla)\mathfrak G(\boldsymbol r,\boldsymbol r')][(\boldsymbol n'\cdot\nabla')\mathfrak G(\boldsymbol r,\boldsymbol r')]\,\mathrm dS'$$

is finite for every $\boldsymbol r\in\partial V$, it is then evident that the double surface integral in Eq. 7 converges. Hence, we have established the Hilbert-Schmidt bound $\|(\hat I+2\hat{\mathscr G}-2\hat\gamma)^2(\hat{\mathscr G}-\hat\gamma)\|_2<+\infty$. ∎

Remark In the course of this proof, the expression in Eq. 7 provides a (theoretically) computable upper bound for $\|(\hat I+2\hat{\mathscr G}-2\hat\gamma)^2(\hat{\mathscr G}-\hat\gamma)\|_2$. For an arbitrary shape $V\Subset\mathbb R^3$, this eventually boils down to a quadruple surface integral of purely geometric quantities:

$$\begin{aligned}&\oiint_{\partial V}\left\{\oiint_{\partial V}[(\boldsymbol n\cdot\nabla)\mathfrak G(\boldsymbol r,\boldsymbol r')][(\boldsymbol n'\cdot\nabla')\mathfrak G(\boldsymbol r,\boldsymbol r')]\,\mathrm dS'\right\}\mathrm dS\\&=\oiint_{\partial V}\mathrm dS_1\oiint_{\partial V}\mathrm dS_2\oiint_{\partial V}\mathrm dS_3\oiint_{\partial V}\mathrm dS_4\prod_{j=1}^4\left[\frac{\boldsymbol n_j\cdot(\boldsymbol r_j-\boldsymbol r_{j+1\bmod 4})}{2\pi|\boldsymbol r_j-\boldsymbol r_{j+1\bmod 4}|^3}-\frac{1}{\oiint_{\partial V}\mathrm dS_j}\right],\end{aligned}$$

which could be practically challenging in numerical evaluations. In the current work, we will not further discuss the practical computation of the surface integral in Eq. 7, except for a specific example in §4.1 concerning a spherical boundary surface ∂V.

It might appear as an interesting fact that the degree of the Hilbert-Schmidt polynomial $\deg(\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}})^2)=3=\dim\mathbb{R}^3$ equals the dimension of the space where the dielectric volume V resides. This is not a pure coincidence, which we will explain later in §4.3. ∎

4. EXAMPLES AND DISCUSSIONS

4.1. Hilbert-Schmidt Qualifications in Mie Scattering

In the Mie scattering scenario, the dielectric medium occupies a spherical volume $V=O(\mathbf{0},R)$ with radius R. Using spherical harmonics $Y_{\ell m}(\theta,\phi)$, we may verify Theorem 1.2 with brute force, and compare the geometric representation of the Hilbert-Schmidt norm (Eq. 7) with an algebraic approach.

Proposition 4.1 *The operator $\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}})^2:\Phi(O(\mathbf{0},R);\mathbb{C}^3)\longrightarrow\Phi(O(\mathbf{0},R);\mathbb{C}^3)$ is of Hilbert-Schmidt type, while the operator $\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}}):\Phi(O(\mathbf{0},R);\mathbb{C}^3)\longrightarrow\Phi(O(\mathbf{0},R);\mathbb{C}^3)$ is compact, without being a Hilbert-Schmidt operator.*

Moreover, we have the identity

$$\sum_{s=1}^{\infty}\|(\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})^2\boldsymbol{f}_s\|^2_{L^2(O(\mathbf{0},R);\mathbb{C}^3)}=\oiint_{\partial O(\mathbf{0},R)}\left\{\oiint_{\partial O(\mathbf{0},R)}[(\boldsymbol{n}\cdot\nabla)\mathfrak{G}(\boldsymbol{r},\boldsymbol{r}')][(\boldsymbol{n}'\cdot\nabla')\mathfrak{G}(\boldsymbol{r},\boldsymbol{r}')]\,\mathrm{d}S'\right\}\mathrm{d}S=\sum_{\ell=1}^{\infty}\frac{1}{(2\ell+1)^3}$$

for any complete orthonormal basis $\{\boldsymbol{f}_s|s=1,2,\dots\}$ of $\Phi(O(\mathbf{0},R);\mathbb{C}^3)$.

Proof It would suffice to check the first two claims on the operator polynomials $(\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})^2(\hat{\mathscr{G}}-\hat{\gamma})$ and $(\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})(\hat{\mathscr{G}}-\hat{\gamma})$. According to [Ref. 1, p. 190], we have the spectral decomposition:

$$(\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E}=-\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\frac{\ell\langle\boldsymbol{f}_{\ell m},\boldsymbol{E}\rangle_{O(\mathbf{0},R)}\boldsymbol{f}_{\ell m}}{2\ell+1},\quad\forall\boldsymbol{E}\in\Phi(O(\mathbf{0},R);\mathbb{C}^3),$$

with the complete orthonormal basis set $\{\boldsymbol{f}_{\ell m}(\boldsymbol{r})=(\ell R^{2\ell+1})^{-1/2}\nabla(|\boldsymbol{r}|^{\ell}Y_{\ell m}(\theta,\phi))|\ell=1,2,\dots;m=[-\ell,\ell]\cap\mathbb{Z}\}$ for $\mathrm{Cl}((\hat{\mathscr{G}}-\hat{\gamma})\Phi(O(\mathbf{0},R);\mathbb{C}^3))$.

By definition of the Hilbert-Schmidt norm, we may compute

$$\|(\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})^2(\hat{\mathscr{G}}-\hat{\gamma})\|_2=\sqrt{\sum_{\ell=1}^{\infty}\frac{\ell^2}{(2\ell+1)^5}}<+\infty,$$

so $(\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})^2(\hat{\mathscr{G}}-\hat{\gamma}):\Phi(O(\mathbf{0},R);\mathbb{C}^3)\longrightarrow\Phi(O(\mathbf{0},R);\mathbb{C}^3)$ is a Hilbert-Schmidt operator.

Meanwhile, the spectral decomposition

$$(\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})(\hat{\mathscr{G}}-\hat{\gamma})\boldsymbol{E}=-\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\frac{\ell\langle\boldsymbol{f}_{\ell m},\boldsymbol{E}\rangle_V\boldsymbol{f}_{\ell m}}{(2\ell+1)^2},\quad\forall\boldsymbol{E}\in\Phi(O(\mathbf{0},R);\mathbb{C}^3)$$

tells us that the operator $(\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})(\hat{\mathscr{G}}-\hat{\gamma}):\Phi(O(\mathbf{0},R);\mathbb{C}^3)\longrightarrow\Phi(O(\mathbf{0},R);\mathbb{C}^3)$ is the uniform limit of a sequence of finite-rank operators, hence compact. However, this compact operator fails the Hilbert-Schmidt criterion because

$$\|(\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})(\hat{\mathscr{G}}-\hat{\gamma})\|_2=\sqrt{\sum_{\ell=1}^{\infty}\frac{\ell^2}{(2\ell+1)^3}}=+\infty.$$

This stark contrast reveals that the additional factor $(\hat{I}+2\hat{\mathscr{G}})$ plays an indispensable rôle in turning a compact operator $\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}})$ into a Hilbert-Schmidt operator $\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}})^2$.

From an algebraic perspective, we doubtlessly have

$$\sum_{s=1}^{\infty}\|(\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})^2\boldsymbol{f}_s\|^2_{L^2(O(\mathbf{0},R);\mathbb{C}^3)}=\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\|(\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})^2\boldsymbol{f}_{\ell m}\|^2_{L^2(O(\mathbf{0},R);\mathbb{C}^3)}=\sum_{\ell=1}^{\infty}\frac{1}{(2\ell+1)^3}.$$

However, we may also compute the Hilbert-Schmidt norm by explicitly evaluating the geometric integral (Eq. 7), with the help of spherical harmonics. Concretely, we have

$$\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}=-2R\boldsymbol{n}\cdot\nabla\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}=2R\frac{\boldsymbol{n}\cdot(\boldsymbol{r}-\boldsymbol{r}')}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|^3}=\frac{1}{R}\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{1}{2\ell+1}Y^*_{\ell m}(\theta,\phi)Y_{\ell m}(\theta',\phi'),\quad |\boldsymbol{r}|=|\boldsymbol{r}'|=R,$$

according to the simple algebra $2R\boldsymbol{n}\cdot(\boldsymbol{r}-\boldsymbol{r}')=\boldsymbol{r}\cdot\boldsymbol{r}-2\boldsymbol{r}\cdot\boldsymbol{r}'+\boldsymbol{r}'\cdot\boldsymbol{r}'=|\boldsymbol{r}-\boldsymbol{r}'|^2$ for $\boldsymbol{r},\boldsymbol{r}'\in\partial V=\partial O(\mathbf{0},R)$. This leads to the calculation

$$\begin{aligned}(\boldsymbol{n}\cdot\nabla)\mathfrak{G}(\boldsymbol{r},\boldsymbol{r}')&=\frac{1}{4\pi^2}\oiint_{\partial O(\mathbf{0},R)}\left[\frac{\boldsymbol{n}\cdot(\boldsymbol{r}-\boldsymbol{r}'')}{|\boldsymbol{r}-\boldsymbol{r}''|^3}-\frac{1}{2R^2}\right]\left[\frac{\boldsymbol{n}''\cdot(\boldsymbol{r}''-\boldsymbol{r})}{|\boldsymbol{r}''-\boldsymbol{r}'|^3}-\frac{1}{2R^2}\right]\mathrm{d}S''\\&=\frac{1}{R^2}\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\frac{1}{(2\ell+1)^2}Y^*_{\ell m}(\theta,\phi)Y_{\ell m}(\theta',\phi')=(\boldsymbol{n}'\cdot\nabla')\mathfrak{G}(\boldsymbol{r},\boldsymbol{r}'),\end{aligned}$$

and consequently Eq. 7 can be computed as

$$\oiint_{\partial O(\mathbf{0},R)}\left\{\oiint_{\partial O(\mathbf{0},R)}[(\boldsymbol{n}\cdot\nabla)\mathfrak{G}(\boldsymbol{r},\boldsymbol{r}')][(\boldsymbol{n}'\cdot\nabla')\mathfrak{G}(\boldsymbol{r},\boldsymbol{r}')]\,\mathrm{d}S'\right\}\mathrm{d}S=\sum_{\ell=1}^{\infty}\frac{1}{(2\ell+1)^3}=\frac{7\zeta(3)}{8}-1.$$

While it becomes impractical to algebraically enumerate all the eigenvectors of the operator $\hat{\mathscr{G}}-\hat{\gamma}$ for non-spherical shapes, we may still fall back on the geometric integral representation (Eq. 7) to deduce a finite Hilbert-Schmidt norm from the bounded curvatures of the smooth boundary ∂V. ∎

Remark For the sphere with radius R, the Green function with Dirichlet boundary condition can be developed into the following spherical harmonic series [Ref. 6, p. 65]:

$$\begin{aligned}G_D(\boldsymbol{r},\boldsymbol{r}')&=\frac{1}{4\pi\max(|\boldsymbol{r}|,|\boldsymbol{r}'|)}-\frac{1}{4\pi R}+\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\frac{Y^*_{\ell m}(\theta,\phi)Y_{\ell m}(\theta',\phi')}{(2\ell+1)\max(|\boldsymbol{r}|,|\boldsymbol{r}'|)}\left\{\left[\frac{\min(|\boldsymbol{r}|,|\boldsymbol{r}'|)}{\max(|\boldsymbol{r}|,|\boldsymbol{r}'|)}\right]^{\ell}-\frac{|\boldsymbol{r}|^{\ell}|\boldsymbol{r}'|^{\ell}\max(|\boldsymbol{r}|,|\boldsymbol{r}'|)}{R^{2\ell+1}}\right\}\\&=\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}-\frac{1}{4\pi R}-\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\frac{|\boldsymbol{r}|^{\ell}|\boldsymbol{r}'|^{\ell}Y^*_{\ell m}(\theta,\phi)Y_{\ell m}(\theta',\phi')}{(2\ell+1)R^{2\ell+1}}.\end{aligned}$$

Meanwhile, the symmetrized Green function with Neumann boundary condition has an explicit series representation [Ref. 6, p. 144]:

$$\begin{aligned}G_N(\boldsymbol{r},\boldsymbol{r}')&=\frac{1}{4\pi\max(|\boldsymbol{r}|,|\boldsymbol{r}'|)}+\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\frac{Y^*_{\ell m}(\theta,\phi)Y_{\ell m}(\theta',\phi')}{(2\ell+1)\max(|\boldsymbol{r}|,|\boldsymbol{r}'|)}\left\{\left[\frac{\min(|\boldsymbol{r}|,|\boldsymbol{r}'|)}{\max(|\boldsymbol{r}|,|\boldsymbol{r}'|)}\right]^{\ell}+\frac{\ell+1}{\ell}\frac{|\boldsymbol{r}|^{\ell}|\boldsymbol{r}'|^{\ell}\max(|\boldsymbol{r}|,|\boldsymbol{r}'|)}{R^{2\ell+1}}\right\}\\&=\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}+\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\frac{\ell+1}{\ell}\frac{|\boldsymbol{r}|^{\ell}|\boldsymbol{r}'|^{\ell}Y^*_{\ell m}(\theta,\phi)Y_{\ell m}(\theta',\phi')}{(2\ell+1)R^{2\ell+1}}.\end{aligned}$$

It is then clear that

$$\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}'):=G_D(\boldsymbol{r},\boldsymbol{r}')+G_N(\boldsymbol{r},\boldsymbol{r}')-\frac{1}{2\pi|\boldsymbol{r}-\boldsymbol{r}'|}=-\frac{1}{4\pi R}+\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\frac{|\boldsymbol{r}|^{\ell}|\boldsymbol{r}'|^{\ell}Y^*_{\ell m}(\theta,\phi)Y_{\ell m}(\theta',\phi')}{\ell(2\ell+1)R^{2\ell+1}}$$

provides yet another means to solve the eigenvalue problem

$$((\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})\boldsymbol{F}_\lambda)(\boldsymbol{r})=\iiint_{O(\mathbf{0},R)}\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\cdot\boldsymbol{F}_\lambda(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}'=\lambda\boldsymbol{F}_\lambda(\boldsymbol{r}),\quad \boldsymbol{F}_\lambda\in\Phi(O(\mathbf{0},R);\mathbb{C}^3).$$

Furthermore, the series representation of $\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$ can be summed into

$$\begin{aligned}\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')+\frac{1}{4\pi R}&=\int_0^1\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\frac{t^{\ell-1}|\boldsymbol{r}|^{\ell}|\boldsymbol{r}'|^{\ell}Y^*_{\ell m}(\theta,\phi)Y_{\ell m}(\theta',\phi')}{(2\ell+1)R^{2\ell+1}}\,\mathrm{d}t=\int_0^1\left(\left|\frac{\boldsymbol{r}}{|\boldsymbol{r}|}-\frac{t|\boldsymbol{r}||\boldsymbol{r}'|}{R^2}\frac{\boldsymbol{r}'}{|\boldsymbol{r}'|}\right|^{-1}-1\right)\frac{\mathrm{d}t}{4\pi Rt}\\&=\frac{1}{4\pi R}\ln\frac{2}{1-\frac{\boldsymbol{r}\cdot\boldsymbol{r}'}{R^2}+\left|\frac{\boldsymbol{r}}{|\boldsymbol{r}|}-\frac{|\boldsymbol{r}||\boldsymbol{r}'|}{R^2}\frac{\boldsymbol{r}'}{|\boldsymbol{r}'|}\right|}.\end{aligned}$$

Thus, there is a mild logarithmic divergence $\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')=O(\ln|\boldsymbol{r}-\boldsymbol{r}'|)$ if at least one of $\boldsymbol{r}$ and $\boldsymbol{r}'$ is situated on the spherical boundary $\partial O(\mathbf{0},R)$. Overall, the singular part of $\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$ has order $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-2})$. Such asymptotic behavior is not a trend specific to spherical geometry, but a generic property descending from the curvature bounds of the boundary surface ∂V (see §4.3).

Owing to the bound $\|\hat{\mathscr{G}}-\hat{\gamma}\|\leq 1/2$ in the spherical case, the Hilbert-Schmidt norm estimate in Eq. 5 does allow a modest improvement in the case of Mie scattering:

$$\begin{aligned}
&\|(\hat I+2\hat{\mathscr{G}})^2\hat{\mathscr{G}}\|_2\\
\leq{}&\|(\hat I+2\hat{\mathscr{G}}-2\hat\gamma)^2(\hat{\mathscr{G}}-\hat\gamma)\|_2\\
&+\|\hat\gamma+4[(\hat{\mathscr{G}}-\hat\gamma)\hat\gamma+\hat\gamma(\hat{\mathscr{G}}-\hat\gamma)](\hat I+\hat{\mathscr{G}}-\hat\gamma)+4(\hat{\mathscr{G}}-\hat\gamma)^2\hat\gamma+4(\hat I+\hat{\mathscr{G}}-\hat\gamma)\hat\gamma^2+4\hat\gamma(\hat{\mathscr{G}}-\hat\gamma)\hat\gamma+4\hat\gamma^2(\hat{\mathscr{G}}-\hat\gamma)^2+4\hat\gamma^3\|_2\\
\leq{}&\sqrt{\sum_{\ell=1}^\infty\frac{\ell^2}{(2\ell+1)^5}}+\|\hat\gamma\|_2(6+7\|\hat\gamma\|+4\|\hat\gamma\|^2).
\end{aligned}$$

Here, the infinite series in question evaluates to a small number

$$\sum_{\ell=1}^\infty\frac{\ell^2}{(2\ell+1)^5}=\frac{7\zeta(3)}{32}+\frac{31\zeta(5)}{128}-\frac{\pi^4}{192}=(0.0821+)^2,$$

and the upper bounds of $\|\hat\gamma\|_2$ and $\|\hat\gamma\|$ will be given in the next subsection, in a more general geometric context. ∎

4.2. Bounds of Spectral Series in Arbitrarily Shaped Dielectrics

In this subsection, we will describe the bound estimates of $\|\hat\gamma\|$ and $\|\hat\gamma\|_2$ for dielectric media with arbitrary geometry. Combining these estimates with Eq. 7, we will arrive at a theoretical upper bound for the convergent spectral series $\sum_{\lambda\in\sigma^\Phi(\hat{\mathscr{G}})}|\lambda|^2|1+2\lambda|^4$.

In [Ref. 1, pp. 261-272], we established the following bound for $\|\hat\gamma\|$.

Proposition 4.2 *For a bounded open dielectric volume V with smooth boundary ∂V, we have*

$$\max_{\lambda\in\sigma^\Phi(\hat{\mathscr{G}})}|\operatorname{Re}\lambda|\leq 1+\|\operatorname{Re}\hat\gamma\|\leq 1+\min\left\{\frac{3}{5\pi}\left(k^3\iiint_V \mathrm{d}^3\boldsymbol{r}\right)^{2/3},3\sqrt2 kR_V\right\},$$

$$-\min_{\lambda\in\sigma^\Phi(\hat{\mathscr{G}})}\operatorname{Im}\lambda=\max_{\lambda\in\sigma^\Phi(\hat{\mathscr{G}})}|\operatorname{Im}\lambda|\leq\|\operatorname{Im}\hat\gamma\|\leq\min\left\{\frac{k^3}{4\pi}\iiint_V\mathrm{d}^3\boldsymbol{r},\frac{3}{5\pi}\left(k^3\iiint_V \mathrm{d}^3\boldsymbol{r}\right)^{2/3},\frac58 kR_V\right\},$$

and

$$\|\hat\gamma\|\leq\min\left\{\frac{3}{5\pi}\left(k^3\iiint_V \mathrm{d}^3\boldsymbol{r}\right)^{2/3},3\sqrt2 kR_V\right\}+\min\left\{\frac{k^3}{4\pi}\iiint_V\mathrm{d}^3\boldsymbol{r},\frac{3}{5\pi}\left(k^3\iiint_V \mathrm{d}^3\boldsymbol{r}\right)^{2/3},\frac58 kR_V\right\},$$

where $R_V:=\min_{\boldsymbol{r}\in\mathbb{R}^3}\max_{\boldsymbol{r}'\in V\cup\partial V}|\boldsymbol{r}'-\boldsymbol{r}|$ is the minimal radius of all the circumscribed spheres. ∎

Now, we will turn to provide an upper bound for the Hilbert-Schmidt norm $\|\hat\gamma\|_2$.

Proposition 4.3 *For arbitrarily shaped bounded open dielectric volume V, we have*

$$\|\hat\gamma\|_2\leq\min\left\{\frac{2}{\pi}\left(k^3\iiint_V \mathrm{d}^3\boldsymbol{r}\right)^{2/3},\frac32(kR_V)^2\right\},$$

where R_V is the minimal radius of all the circumscribed spheres.

To prove Proposition 4.3, we need some preparations. First, we turn Eq. 2 into the following integral representation

$$(\hat\gamma\boldsymbol{E})(\boldsymbol{r}):=\iiint_V\hat\Gamma(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{E}(\boldsymbol{r}')\mathrm{d}^3\boldsymbol{r}'$$

where the 3×3 matrix $\hat\Gamma(\boldsymbol{r},\boldsymbol{r}')$ is given by

$$\begin{aligned}\hat\Gamma(\boldsymbol{r},\boldsymbol{r}')={}&\frac{k^2}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\left\{\left[e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}+\frac{1-e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}\left(1+ik|\boldsymbol{r}-\boldsymbol{r}'|\right)}{k^2|\boldsymbol{r}-\boldsymbol{r}'|^2}\right]\mathbb{1}\right.\\
&\left.+\left[3\frac{e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}\left(1+ik|\boldsymbol{r}-\boldsymbol{r}'|\right)-1}{k^2|\boldsymbol{r}-\boldsymbol{r}'|^2}-(e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}-1)\right]\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}^{\mathrm{T}}\right\}.\end{aligned}$$

Here,

$$\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}^{\mathrm{T}} = \frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\left(\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\right)^{\mathrm{T}} = (\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}^{\mathrm{T}})^{\mathrm{T}} = \hat{\boldsymbol{r}}\hat{\boldsymbol{r}}^{\mathrm{T}}\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}^{\mathrm{T}}$$

is a projection operator. Then, to facilitate further analysis, we may use the breakdown $\hat{\gamma} = \hat{\gamma}_\sharp + \hat{\gamma}_{\sharp\sharp}$ where

$$(\hat{\gamma}_\sharp \boldsymbol{E})(\boldsymbol{r}) := \iiint_V \hat{\Gamma}_\sharp(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{E}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}' = \iiint_V \frac{k^2}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\left[e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}\mathbb{1} + (1-e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|})\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}^{\mathrm{T}}\right]\boldsymbol{E}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}'$$

and

$$(\hat{\gamma}_{\sharp\sharp} \boldsymbol{E})(\boldsymbol{r}) := \iiint_V \hat{\Gamma}_{\sharp\sharp}(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{E}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}' = \iiint_V \frac{[1-e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}\left(1+ik|\boldsymbol{r}-\boldsymbol{r}'|\right)]}{4\pi k^2|\boldsymbol{r}-\boldsymbol{r}'|^3}\left[\mathbb{1} - 3\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}^{\mathrm{T}}\right]\boldsymbol{E}(\boldsymbol{r}')\,\mathrm{d}^3\boldsymbol{r}'.$$

Lemma 4.1 *The following results hold:*

$$\begin{aligned}
\mathrm{Tr}[\hat{\Gamma}_\sharp^*(\boldsymbol{r},\boldsymbol{r}')\hat{\Gamma}_\sharp(\boldsymbol{r},\boldsymbol{r}')] &= \frac{3k^4}{16\pi^2|\boldsymbol{r}-\boldsymbol{r}'|^2},\\
\mathrm{Tr}[\hat{\Gamma}_{\sharp\sharp}^*(\boldsymbol{r},\boldsymbol{r}')\hat{\Gamma}_{\sharp\sharp}(\boldsymbol{r},\boldsymbol{r}')] &= \frac{3|1-e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}(1+ik|\boldsymbol{r}-\boldsymbol{r}'|)|^2}{8\pi^2|\boldsymbol{r}-\boldsymbol{r}'|^6} \le \frac{3k^4}{32\pi^2|\boldsymbol{r}-\boldsymbol{r}'|^2}.
\end{aligned}$$

Proof We note that for $a,b\in\mathbb{C}$, there is an algebraic identity

$$\mathrm{Tr}[(a\mathbb{1}+b\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}^{\mathrm{T}})^*(a\mathbb{1}+b\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}^{\mathrm{T}})] = \mathrm{Tr}[|a|^2\mathbb{1} + 2\mathrm{Re}(a^*b)\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}^{\mathrm{T}} + |b|^2\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}^{\mathrm{T}}] = 3|a|^2 + 2\mathrm{Re}(a^*b) + |b|^2.$$

In particular, setting $a = e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}$ and $b = 1-e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}$, we have $3|a|^2+2\mathrm{Re}(a^*b)+|b|^2 = 3$; setting $a=1$ and $b=-3$, we have $3|a|^2+2\mathrm{Re}(a^*b)+|b|^2 = 6$. For $x>0$, we have $|e^{ix}-1-ix| \le x^2/2$, which confirms that $\mathrm{Tr}[\hat{\Gamma}_{\sharp\sharp}^*(\boldsymbol{r},\boldsymbol{r}')\hat{\Gamma}_{\sharp\sharp}(\boldsymbol{r},\boldsymbol{r}')] \le \mathrm{Tr}[\hat{\Gamma}_\sharp^*(\boldsymbol{r},\boldsymbol{r}')\hat{\Gamma}_\sharp(\boldsymbol{r},\boldsymbol{r}')]/2$. ∎

Now we may turn to consider the functional

$$I[V] = \sqrt{\iiint_V \left\{\iiint_V \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^2}\,\mathrm{d}^3\boldsymbol{r}'\right\}\mathrm{d}^3\boldsymbol{r}},$$

so that we have the Hilbert-Schmidt bounds

$$\|\hat{\gamma}_\sharp\|_2 \le \sqrt{\iiint_V \left\{\iiint_V \mathrm{Tr}[\hat{\Gamma}_\sharp^*(\boldsymbol{r},\boldsymbol{r}')\hat{\Gamma}_\sharp(\boldsymbol{r},\boldsymbol{r}')]\,\mathrm{d}^3\boldsymbol{r}'\right\}\mathrm{d}^3\boldsymbol{r}} = \frac{\sqrt{3}k^2}{4\pi}I[V],$$

and

$$\|\hat{\gamma}_{\sharp\sharp}\|_2 \le \sqrt{\iiint_V \left\{\iiint_V \mathrm{Tr}[\hat{\Gamma}_{\sharp\sharp}^*(\boldsymbol{r},\boldsymbol{r}')\hat{\Gamma}_{\sharp\sharp}(\boldsymbol{r},\boldsymbol{r}')]\,\mathrm{d}^3\boldsymbol{r}'\right\}\mathrm{d}^3\boldsymbol{r}} \le \frac{\sqrt{6}k^2}{8\pi}I[V].$$

As a result of triangle inequality for the Hilbert-Schmidt norm, we obtain

$$\|\hat{\gamma}\|_2 \le \|\hat{\gamma}_\sharp\|_2 + \|\hat{\gamma}_{\sharp\sharp}\|_2 \le \frac{(2\sqrt{3}+\sqrt{6})k^2}{8\pi}I[V].$$

Lemma 4.2 *We have*

$$I[V] \le \left(\sqrt{2}\pi\iiint_V \mathrm{d}^3\boldsymbol{r}\right)^{2/3}$$

and consequently, we have $\|\hat{\gamma}\|_2 \le (2/\pi)\left(k^3\iiint_V \mathrm{d}^3\boldsymbol{r}\right)^{2/3}$.

Proof Using the Hardy-Littlewood-Sobolev inequality [Refs. 12–14] with Lieb's sharp constant (see [Ref. 15], as well as [Ref. 16, Theorem 4.3]):

$$\left|\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\frac{f(\boldsymbol{r}')h(\boldsymbol{r})}{|\boldsymbol{r}-\boldsymbol{r}'|^m}\mathrm{d}^d\boldsymbol{r}'\,\mathrm{d}^d\boldsymbol{r}\right|\le\pi^{m/2}\frac{\Gamma(\frac{d-m}{2})}{\Gamma(d-\frac{m}{2})}\left[\frac{\Gamma(\frac{d}{2})}{\Gamma(d)}\right]^{-1+\frac{m}{d}}\|f\|_{L^{2d/(2d-m)}(\mathbb{R}^d;\mathbb{C})}\|h\|_{L^{2d/(2d-m)}(\mathbb{R}^d;\mathbb{C})},$$

$$\text{where } d=3, m=2, \frac{2d}{2d-m}=\frac{3}{2};\quad f(\boldsymbol{r})=h(\boldsymbol{r})=\begin{cases}1, & \boldsymbol{r}\in V\\ 0, & \boldsymbol{r}\notin V\end{cases},$$

we may arrive at the following estimate

$$(I[V])^2=\iiint_V\left\{\iiint_V\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^2}\mathrm{d}^3\boldsymbol{r}'\right\}\mathrm{d}^3\boldsymbol{r}\le\left(\sqrt{2}\pi\iiint_V\mathrm{d}^3\boldsymbol{r}\right)^{4/3}.$$

Accordingly, the estimates on $\|\hat{\gamma}\|_2$ derives from $1.997+=(2\sqrt{3}+\sqrt{6})(\sqrt{2}\pi)^{2/3}/8\le 2$. ∎

Remark From this lemma, we have $I[O(\mathbf{0},R)]/R^2\le 7.022+$, which may be compared to the exact value $I[O(\mathbf{0},R)]/R^2=2\pi$ obtained in the next lemma. ∎

Lemma 4.3 *We have*

$$I[V]=\sqrt{\iiint_{\mathbb{R}^3}\frac{|\iiint_V e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\,\mathrm{d}^3\boldsymbol{r}|^2}{4\pi|\boldsymbol{q}|}\mathrm{d}^3\boldsymbol{q}}$$

and in particular, we have the identity $I[O(\mathbf{0},R)]=2\pi R^2$ *for all* $R>0$, *and* $\|\hat{\gamma}\|_2\le\frac{3}{2}(kR_V)^2$.

Proof We start with the Fourier inversion formula

$$\iiint_V\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^2}\mathrm{d}^3\boldsymbol{r}'=\frac{1}{(2\pi)^3}\iiint_{\mathbb{R}^3}\frac{2\pi^2\iiint_V e^{i\boldsymbol{q}\cdot\boldsymbol{r}'}\,\mathrm{d}^3\boldsymbol{r}'}{|\boldsymbol{q}|}e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\,\mathrm{d}^3\boldsymbol{q}$$

where the convolution kernel satisfies

$$\lim_{\varepsilon\to0^+}\iiint_{\mathbb{R}^3}\frac{e^{-\varepsilon|\boldsymbol{r}|}}{|\boldsymbol{r}|^2}e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\,\mathrm{d}^3\boldsymbol{r}=4\pi\lim_{\varepsilon\to0^+}\int_0^{+\infty}\frac{e^{-\varepsilon|\boldsymbol{r}|}\sin(|\boldsymbol{q}||\boldsymbol{r}|)}{|\boldsymbol{q}||\boldsymbol{r}|}\mathrm{d}|\boldsymbol{r}|=\frac{2\pi^2}{|\boldsymbol{q}|}.$$

Then, applying the Parseval-Plancherel identity, we obtain the Fourier representation of $I[V]$ as claimed.

For $V=O(\mathbf{0},R)$, we have

$$\iiint_{V=O(\mathbf{0},R)}e^{i\boldsymbol{q}\cdot\boldsymbol{r}'}\,\mathrm{d}^3\boldsymbol{r}'=4\pi\frac{\sin(|\boldsymbol{q}|R)-|\boldsymbol{q}|R\cos(|\boldsymbol{q}|R)}{|\boldsymbol{q}|^3}=4\pi R^3\frac{j_1(|\boldsymbol{q}|R)}{|\boldsymbol{q}|R},$$

where $j_1(x)$ is the spherical Bessel function of first order. Consequently, we may derive $I[O(\mathbf{0},R)]=2\pi R^2$ from the identity $\int_0^{+\infty}j_1^2(x)/x\,\mathrm{d}x=1/4$, which is a specific case of the Weber-Schafheitlin integral [Ref. 17, pp. 402-404]. We may check this against the spherical harmonic expansion

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^2}=\left|4\pi\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\frac{Y^*_{\ell m}(\theta,\phi)Y_{\ell m}(\theta',\phi')}{(2\ell+1)\max(|\boldsymbol{r}|,|\boldsymbol{r}'|)}\left[\frac{\min(|\boldsymbol{r}|,|\boldsymbol{r}'|)}{\max(|\boldsymbol{r}|,|\boldsymbol{r}'|)}\right]^{\ell}\right|^2,$$

which integrates to

$$\begin{aligned}\iiint_{O(\mathbf{0},R)}\left\{\iiint_{O(\mathbf{0},R)}\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^2}\mathrm{d}^3\boldsymbol{r}'\right\}\mathrm{d}^3\boldsymbol{r}&=(4\pi)^2\sum_{\ell=0}^{\infty}\frac{1}{(2\ell+1)}\int_0^R\left\{\int_0^R\frac{[\min(|\boldsymbol{r}|,|\boldsymbol{r}'|)]^{2\ell}}{[\max(|\boldsymbol{r}|,|\boldsymbol{r}'|)]^{2\ell+2}}|\boldsymbol{r}'|^2\,\mathrm{d}|\boldsymbol{r}'|\right\}|\boldsymbol{r}|^2\,\mathrm{d}|\boldsymbol{r}|\\&=(4\pi)^2R^4\sum_{\ell=0}^{\infty}\frac{1}{2(2\ell+1)(2\ell+3)}=(2\pi R^2)^2.\end{aligned}$$

Suppose that we have chosen the origin $\boldsymbol{r}=\mathbf{0}$ of the coordinate system to coincide with the center of the circumscribed sphere of radius R_V, then we have the relations $V\subset O(\mathbf{0},R_V)$, $I[V]\le I[O(\mathbf{0},R_V)]$, and this eventually establishes $\|\hat{\gamma}\|_2\le(2\sqrt{3}+\sqrt{6})(kR_V)^2/4\le\frac{3}{2}(kR_V)^2$. ∎

So far, we have verified Proposition 4.3 in its entirety. We may check the reasonability of the estimates in Propositions 4.2 and 4.3 by revisiting to the spectral series for Mie scattering on a dielectric with radius R in the short-wavelength limit $kR \to +\infty$:

$$\sum_{\lambda\in\sigma^{\Phi}(\hat{\mathscr{G}})} |\lambda|^2|1+2\lambda|^4 \lesssim \|\hat{\gamma}\|_2^2\|2\hat{\gamma}\|^4 = O(k^8R^8).$$

Here, the $O(k^8R^8)$ behavior can also be recovered from the left-hand side. In the short-wavelength limit, the dominant contributions to the spectral series $\sum_{\lambda\in\sigma^{\Phi}(\hat{\mathscr{G}})}|\lambda|^2|1+2\lambda|^4$ would arise from the eigenvalues associated with $Y_{\ell m}$ modes for $\ell \lesssim kR$. Each such eigenvalue has order $O(kR)$ in magnitude, and there are about $O(k^2R^2)$ terms of them, counting multiplicities. Therefore, the spectral series $\sum_{\lambda\in\sigma^{\Phi}(\hat{\mathscr{G}})}|\lambda|^2|1+2\lambda|^4 = O(k^8R^8)$ is roughly the sum of $O(k^2R^2)$ addends, each with magnitude $O(k^6R^6)$.

Even for non-spherical dielectrics, the consistency of $\sum_{\lambda\in\sigma^{\Phi}(\hat{\mathscr{G}})}|\lambda|^2|1+2\lambda|^4 \lesssim \|\hat{\gamma}\|_2^2\|2\hat{\gamma}\|^4$ in the short-wavelength limit is ready to check. As $\|\hat{\mathscr{G}}-\hat{\gamma}\| \le 1$ remains bounded irrespective of wavelength, we may pretend that the spectra $\sigma^{\Phi}(\hat{\mathscr{G}})$ and $\sigma^{\Phi}(\hat{\gamma})$ are close to each other in the short-wavelength limit, so that we have the following intuitive estimates:

$$\sum_{\lambda\in\sigma^{\Phi}(\hat{\mathscr{G}})} |\lambda|^2|1+2\lambda|^4 \approx \sum_{\lambda'\in\sigma^{\Phi}(\hat{\gamma})} |\lambda'|^2|2\lambda'|^4 \le \|2\hat{\gamma}\|^4 \sum_{\lambda'\in\sigma^{\Phi}(\hat{\gamma})} |\lambda'|^2 \le \|\hat{\gamma}\|_2^2\|2\hat{\gamma}\|^4.$$

4.3. Comparison with Acoustic Scattering and Low-Dimensional Electromagnetic Scattering

The analytic peculiarity of electromagnetic scattering problems can be better appreciated if we contrast it to the scattering problems concerning scalar acoustic waves in spatial dimensions $d = 1,2,3$.

For example, the acoustic scattering equation in three-dimensional space

$$((\hat{I}-\chi\hat{\mathscr{C}})u)(\boldsymbol{r}) := u(\boldsymbol{r}) - \chi\iiint_V \frac{u(\boldsymbol{r}')k^2e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}^3\boldsymbol{r}' = u_{\mathrm{inc}}(\boldsymbol{r}),\quad u_{\mathrm{inc}}\in L^2(V;\mathbb{C})$$

involves a perturbation of the identity operator $\hat{I}$ by a Hilbert-Schmidt operator $-\chi\hat{\mathscr{C}}: L^2(V;\mathbb{C}) \longrightarrow L^2(V;\mathbb{C})$, and thus has significantly simplified spectral properties as compared to the Born equation for light scattering. The integral equation $(\hat{I}-\chi\hat{\mathscr{C}})u = u_{\mathrm{inc}}$ is a Fredholm equation with convergent spectral series $\sum_{\lambda\in\sigma(\hat{\mathscr{C}})}|\lambda|^2 = \sum_{\lambda\in\sigma_p(\hat{\mathscr{C}})}|\lambda|^2 < +\infty$. Such an integral equation admits relatively simple expansion of $(\hat{I}-\chi\hat{\mathscr{C}})^{-1}$ for any $1/\chi \notin \sigma(\hat{\mathscr{C}})$ [see Ref. 10, Chap. 5].

For the scattering of electromagnetic waves, we lack compactness in the Green operator $\hat{\mathscr{G}}: \Phi(V;\mathbb{C}^3) \longrightarrow \Phi(V;\mathbb{C}^3)$, and it takes a quadratic polynomial $\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}}): \Phi(V;\mathbb{C}^3) \longrightarrow \Phi(V;\mathbb{C}^3)$ to recover compactness, a cubic polynomial $\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}})^2$: $\Phi(V;\mathbb{C}^3) \longrightarrow \Phi(V;\mathbb{C}^3)$ to qualify as a Hilbert-Schmidt operator.

Heuristically, we can interpret the compactness of $(\hat{\mathscr{G}}-\hat{\gamma})+2(\hat{\mathscr{G}}-\hat{\gamma})^2 : \Phi(V;\mathbb{C}^3) \longrightarrow \Phi(V;\mathbb{C}^3)$ in terms of an integral kernel $\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$ with $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-2})$ asymptotic behavior, which mitigates the strong singularity of order $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-3})$ associated with the non-compact operator $\hat{\mathscr{G}}$. Here, the harmonic function $\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$ develops singularity as the points $\boldsymbol{r},\boldsymbol{r}'$ approach the dielectric boundary ∂V, and their distance approaches zero $|\boldsymbol{r}-\boldsymbol{r}'| \to 0^+$, so we may sketch the $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-2})$ behavior of the integral kernel $\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$ by focusing on the near-boundary cases.

We choose $\boldsymbol{r}' \in \partial V$ as a boundary point and use $T_{\boldsymbol{r}'}(\partial V)$ to denote the tangent plane of ∂V at the point $\boldsymbol{r}' \in \partial V$, and write $\boldsymbol{n}'$ for the outward unit normal vector at $\boldsymbol{r}'$. We situate the interior point $\boldsymbol{r} = \boldsymbol{r}' - \varepsilon\boldsymbol{n}' \in V$ so close to the boundary point $\boldsymbol{r}'$ that the distance $\varepsilon := |\boldsymbol{r}-\boldsymbol{r}'|$ is negligible as compared to both the characteristic linear dimension ℓ_V of the volume V and the principal radii of curvature at $\boldsymbol{r}' \in \partial V$. The local "surface charge density" $(\boldsymbol{n}_*\cdot\nabla_*)\mathfrak{g}(\boldsymbol{r}_*,\boldsymbol{r}')$ for a

Integral Equation	*Spectral Series*	*Operator*	*Integral Kernel*	*Compact*	*Hilbert-Schmidt*
Electromagnetic Scattering $(\hat{I}-\chi\hat{\mathscr{G}})\boldsymbol{E} = \boldsymbol{E}_{\mathrm{inc}}$	$\hat{\mathscr{G}}: \Phi(V;\mathbb{C}^3) \longrightarrow \Phi(V;\mathbb{C}^3)$ $\sum_{\lambda\in\sigma^{\Phi}(\hat{\mathscr{G}})}|\lambda|^2|1+2\lambda|^4 < +\infty$	$\hat{\mathscr{G}}$	$O(\|\boldsymbol{r}-\boldsymbol{r}'\|^{-3})$	No	No
		$\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}})$	$O(\|\boldsymbol{r}-\boldsymbol{r}'\|^{-2})$	Yes	No
		$\hat{\mathscr{G}}(\hat{I}+2\hat{\mathscr{G}})^2$	$O(\|\boldsymbol{r}-\boldsymbol{r}'\|^{-1})$	Yes	Yes
Acoustic Scattering $(\hat{I}-\chi\hat{\mathscr{C}})u = u_{\mathrm{inc}}$	$\hat{\mathscr{C}}: L^2(V;\mathbb{C}) \longrightarrow L^2(V;\mathbb{C})$ $\sum_{\lambda\in\sigma(\hat{\mathscr{C}})}|\lambda|^2 < +\infty$	$\hat{\mathscr{C}}$	$O(\|\boldsymbol{r}-\boldsymbol{r}'\|^{-1})$	Yes	Yes

Table I A comparison of various operators arising from three-dimensional electromagnetic and acoustic scattering problems, in terms of their asymptotic behavior in the integral kernel, their compactness, and their Hilbert-Schmidt boundedness.

Integral Equation	*Spectral Series*	*Operator*	*Compact*	*Hilbert-Schmidt*
Electromagnetic Scattering $(\hat{I}-\chi\hat{\mathscr{G}}^{(d)})\boldsymbol{E}=\boldsymbol{E}_{\mathrm{inc}}$	$\sum_{\lambda\in\sigma^{\Phi}(\hat{\mathscr{G}}^{(d)})}\lvert\lambda\rvert^2\lvert 1+2\lambda\rvert^{2(d-1)}<+\infty$	$\hat{\mathscr{G}}^{(d)}$	1	1
		$\hat{\mathscr{G}}^{(d)}(\hat{I}+2\hat{\mathscr{G}}^{(d)})$	1,2,3	1,2
		$\hat{\mathscr{G}}^{(d)}(\hat{I}+2\hat{\mathscr{G}}^{(d)})^2$	1,2,3	1,2,3
Acoustic Scattering $(\hat{I}-\chi\hat{\mathscr{C}}^{(d)})u=u_{\mathrm{inc}}$	$\sum_{\lambda\in\sigma(\hat{\mathscr{C}}^{(d)})}\lvert\lambda\rvert^2<+\infty$	$\hat{\mathscr{C}}^{(d)}$	1,2,3	1,2,3

Table II A comparison for the dimension-dependence of the spectral structure in electromagnetic and acoustic scattering problems. The last two columns are filled with spatial dimensions d where the operator in question is compact, or Hilbert-Schmidt.

boundary point $\boldsymbol{r}_*\in\partial V$ near $\boldsymbol{r}'$ has a singular part $\sim\kappa_{\boldsymbol{r}'}/|\boldsymbol{r}_*-\boldsymbol{r}'|$ where $\kappa_{\boldsymbol{r}'}$ is a quantity comparable to the curvature of the surface at point $\boldsymbol{r}'$. The "electrostatic potential" $\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$ thus scales asymptotically as

$$\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')\sim\iint_{T_{\boldsymbol{r}'}(\partial V)\cap O(\boldsymbol{r}',\ell_V)}\frac{\kappa_{\boldsymbol{r}'}\,\mathrm{d}^2(\boldsymbol{r}_*-\boldsymbol{r}')}{4\pi|\boldsymbol{r}_*-\boldsymbol{r}'|\sqrt{\varepsilon^2+|\boldsymbol{r}_*-\boldsymbol{r}'|^2}}=\int_0^{\ell_V}\frac{\kappa_{\boldsymbol{r}'}\,\mathrm{d}\rho}{2\sqrt{\varepsilon^2+\rho^2}}=\frac{\kappa_{\boldsymbol{r}'}}{2}\ln\frac{\ell_V+\sqrt{\varepsilon^2+\ell_V^2}}{h}\approx\frac{\kappa_{\boldsymbol{r}'}}{2}\ln\frac{2\ell_V}{|\boldsymbol{r}-\boldsymbol{r}'|}.$$

This rough estimate hints at the $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-2})$ bound of the integral kernel $\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$, which hearkens back to the spherical example computed in the Remark to Proposition 4.1. Intuitively, one may say that the $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-2})$ bound for the volume integral kernel descends from the boundary integral kernel with $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-1})$ behavior in Proposition 2.1. Such an intuition can be made rigorous for arbitrary boundary geometry, once we work out the compactness proof of Proposition 2.1 in fuller detail in the volume integral setting [Ref. 1, pp. 203-214, pp. 232-246], where the Calderón-Zygmund cancellation conditions [Ref. 18, p. 306 and p. 324] explain the mollification of the strong singularity $O(|\boldsymbol{r}-\boldsymbol{r}|^{-3})$ in the operator polynomial $(\hat{\mathscr{G}}-\hat{\gamma})+2(\hat{\mathscr{G}}-\hat{\gamma})^2$.

Consequently, in view of the integral kernel $\nabla\nabla'\mathfrak{g}(\boldsymbol{r},\boldsymbol{r}')$ with $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-2})$ behavior, along with the identity [Ref. 19, p. 117]

$$\iiint_{\mathbb{R}^3}\frac{1}{2\pi^2|\boldsymbol{r}-\boldsymbol{r}''|^2}\frac{1}{2\pi^2|\boldsymbol{r}''-\boldsymbol{r}'|^2}\mathrm{d}^3\boldsymbol{r}''=\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|},$$

we may envision that the integral kernel corresponding to $(\hat{I}+2\hat{\mathscr{G}}-2\hat{\gamma})^2(\hat{\mathscr{G}}-\hat{\gamma})$ would have $O(|\boldsymbol{r}-\boldsymbol{r}'|^{-1})$ asymptotic behavior, which is square integrable. This gives an intuitive understanding of Theorem 1.2.

Next, we show that the analytic structure of wave scattering not only is affected by degrees of freedom (vector wave *versus* scalar wave), but also dimensionality. We note that the acoustic scattering problem can be formulated in arbitrary spatial dimensions by replacing $V\Subset\mathbb{R}^3$ with a bounded open set $\Omega\Subset\mathbb{R}^d$, and accordingly substituting the integral kernel

$$\frac{k^2e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\quad\text{with}\quad K^{(d)}(\boldsymbol{r},\boldsymbol{r}')=\frac{k^{(d+2)/2}H^{(2)}_{(d-2)/2}(k|\boldsymbol{r}-\boldsymbol{r}'|)}{4i(2\pi|\boldsymbol{r}-\boldsymbol{r}'|)^{(d-2)/2}},$$

where $H^{(2)}_\nu$ denotes the νth order cylindrical Hankel function of the second kind. In particular, $4iK^{(2)}(\boldsymbol{r},\boldsymbol{r}')=k^2H^{(2)}_0(k|\boldsymbol{r}-\boldsymbol{r}'|)=-2ik^2[\ln(k|\boldsymbol{r}-\boldsymbol{r}'|)]/\pi+\mathrm{const}+O(|\boldsymbol{r}-\boldsymbol{r}'|^2\ln(k|\boldsymbol{r}-\boldsymbol{r}'|))$ and $2iK^{(1)}(\boldsymbol{r},\boldsymbol{r}')=ke^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}$. A brute-force computation reveals that the integral kernels $K^{(d)}(\boldsymbol{r},\boldsymbol{r}')$ have finite Hilbert-Schmidt bounds for $d=1,2,3$, so they induce the corresponding Hilbert-Schmidt operators $\hat{\mathscr{C}}^{(d)}$ for acoustic scattering problems. The electromagnetic wave scattering can be modeled in lower spatial dimensions $d=1,2$ by modifying the Born equation into

$$\boldsymbol{E}_{\mathrm{inc}}(\boldsymbol{r})=((\hat{I}-\chi\hat{\mathscr{G}}^{(d)})\boldsymbol{E})(\boldsymbol{r}):=\boldsymbol{E}(\boldsymbol{r})-\chi\int_\Omega\boldsymbol{E}(\boldsymbol{r}')K^{(d)}(\boldsymbol{r},\boldsymbol{r}')\mathrm{d}^d\boldsymbol{r}'-\frac{\chi}{k^2}\nabla\left[\nabla\cdot\int_\Omega\boldsymbol{E}(\boldsymbol{r}')K^{(d)}(\boldsymbol{r},\boldsymbol{r}')\mathrm{d}^d\boldsymbol{r}'\right],\quad\boldsymbol{r}\in\Omega\Subset\mathbb{R}^d.$$

The last term in the above integral equation drops off for $d=1$, so $\hat{\mathscr{G}}^{(1)}$ is a Hilbert-Schmidt operator, just as $\hat{\mathscr{C}}^{(1)}$. For $d=2$, we may define

$$\mathfrak{g}^{(2)}(\boldsymbol{r},\boldsymbol{r}')=G^{(2)}_D(\boldsymbol{r},\boldsymbol{r}')+G^{(2)}_N(\boldsymbol{r},\boldsymbol{r}')-\frac{1}{\pi}\ln\frac{1}{k|\boldsymbol{r}-\boldsymbol{r}'|},$$

and notice that the Hermitian operator induced by the integral kernel $\nabla\nabla'\mathfrak{g}^{(2)}(\boldsymbol{r},\boldsymbol{r}')$ is already of Hilbert-Schmidt type. This is because

$$(\boldsymbol{n}'\cdot\nabla')\mathfrak{g}^{(2)}(\boldsymbol{r},\boldsymbol{r}')=\frac{1}{\pi}(\boldsymbol{n}'\cdot\nabla')\ln\frac{1}{k|\boldsymbol{r}-\boldsymbol{r}'|}+\frac{1}{\oint_{\partial\Omega}\mathrm{d}s'}=\frac{\boldsymbol{n}'\cdot(\boldsymbol{r}-\boldsymbol{r}')}{\pi|\boldsymbol{r}-\boldsymbol{r}'|^2}+\frac{1}{\oint_{\partial\Omega}\mathrm{d}s'},\quad\boldsymbol{r},\boldsymbol{r}'\in\partial\Omega$$

is bounded, provided that the boundary curve $\partial\Omega$ is smooth. Thus, in place of Eq. 7, we have

$$0 \le \oint_{\partial\Omega}\left\{\oint_{\partial\Omega}[(\boldsymbol{n}\cdot\nabla)\mathfrak{g}^{(2)}(\boldsymbol{r},\boldsymbol{r}')][(\boldsymbol{n}'\cdot\nabla')\mathfrak{g}^{(2)}(\boldsymbol{r},\boldsymbol{r}')]\,\mathrm{d}s'\right\}\mathrm{d}s < +\infty,$$

leading to the conclusion that the quadratic polynomial $\hat{\mathscr{G}}^{(2)}(\hat I + 2\hat{\mathscr{G}}^{(2)})$ is a Hilbert-Schmidt operator. In summary, $\hat{\mathscr{G}}^{(d)}(\hat I + 2\hat{\mathscr{G}}^{(d)})^{d-1}$ is a Hilbert-Schmidt polynomial of degree d for spatial dimensions $d = 1, 2, 3$.

We have tabulated the different aspects of analytic behavior for three-dimensional electromagnetic (vector wave) and acoustic (scalar wave) scattering in Table I, and compare the dimension-dependence of the two types of scattering problems in Table II. It might be noted that despite the drastically different analytic properties between these two types of scattering problems, the scalar wave approximation is still a popular approach to the treatment of interactions between light and "objects much larger than wavelength", such as in the scalar diffraction theory [Ref. 6, pp. 478-482]. This is not particularly surprising as the overall spectral behavior of $\hat{\mathscr{G}}$ can be very close to that of a Hilbert-Schmidt operator $\hat\gamma$ in the short-wavelength limit (cf. the discussion of spectral series $\sum_{\lambda\in\sigma^{\Phi}(\hat{\mathscr{G}})}|\lambda|^2|1+2\lambda|^4$ in §4.2).

However, the goodness of approximation generated from scalar wave models of light-matter interaction cannot be taken for granted in all scenarios. We caution that for dimensions $d = 2$ and 3, there are some practically relevant regimes ("large wavelength" [20, 21], "small particle" [22, 23]) where the salient contributions to the spectrum $\sigma^{\Phi}(\hat{\mathscr{G}})$ come from two sequences of points aggregating around the points $\{0\}$ and $\{-1/2\}$. The latter sequence points to a universal resonance mode $1/\chi = -1/2$ (i.e $\epsilon_r = -1$) that attracts scattering eigenvalues, which is a property intrinsic to electromagnetic scattering, unfound in scalar wave phenomena.

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